wwPDB X-ray Structure Validation Summary Report (i)

Apr 25, 2022 – 07:05 pm BST

PDB ID	:	2IUK
Title	:	Crystal structure of Soybean Lipoxygenase-D
Authors	:	Youn, B.; Sellhorn, G.E.; Mirchel, R.J.; Gaffney, B.J.; Grimes, H.D.; Kang, C.
Deposited on	:	2006-06-05
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

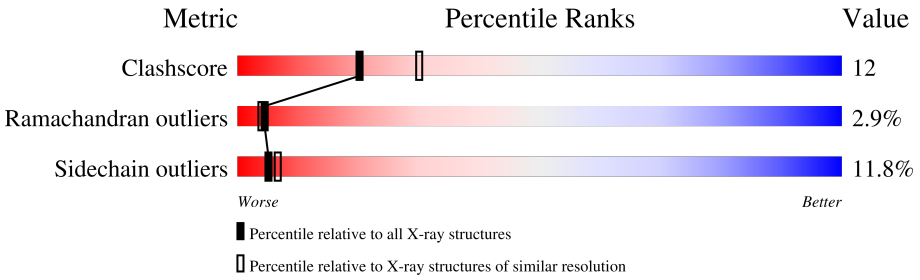
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	864	60% 29% 7%
1	B	864	59% 30% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13534 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SEED LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			
1	B	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	PHE	LEU	conflict	UNP P24095
A	233	CYS	SER	conflict	UNP P24095
A	240	LEU	ARG	conflict	UNP P24095
A	364	VAL	TRP	conflict	UNP P24095
A	604	HIS	ASP	conflict	UNP P24095
A	695	LYS	MET	conflict	UNP P24095
B	1192	PHE	LEU	conflict	UNP P24095
B	1233	CYS	SER	conflict	UNP P24095
B	1240	LEU	ARG	conflict	UNP P24095
B	1364	VAL	TRP	conflict	UNP P24095
B	1604	HIS	ASP	conflict	UNP P24095
B	1695	LYS	MET	conflict	UNP P24095

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	121	Total O 121 121	0	0
3	B	113	Total O 113 113	0	0

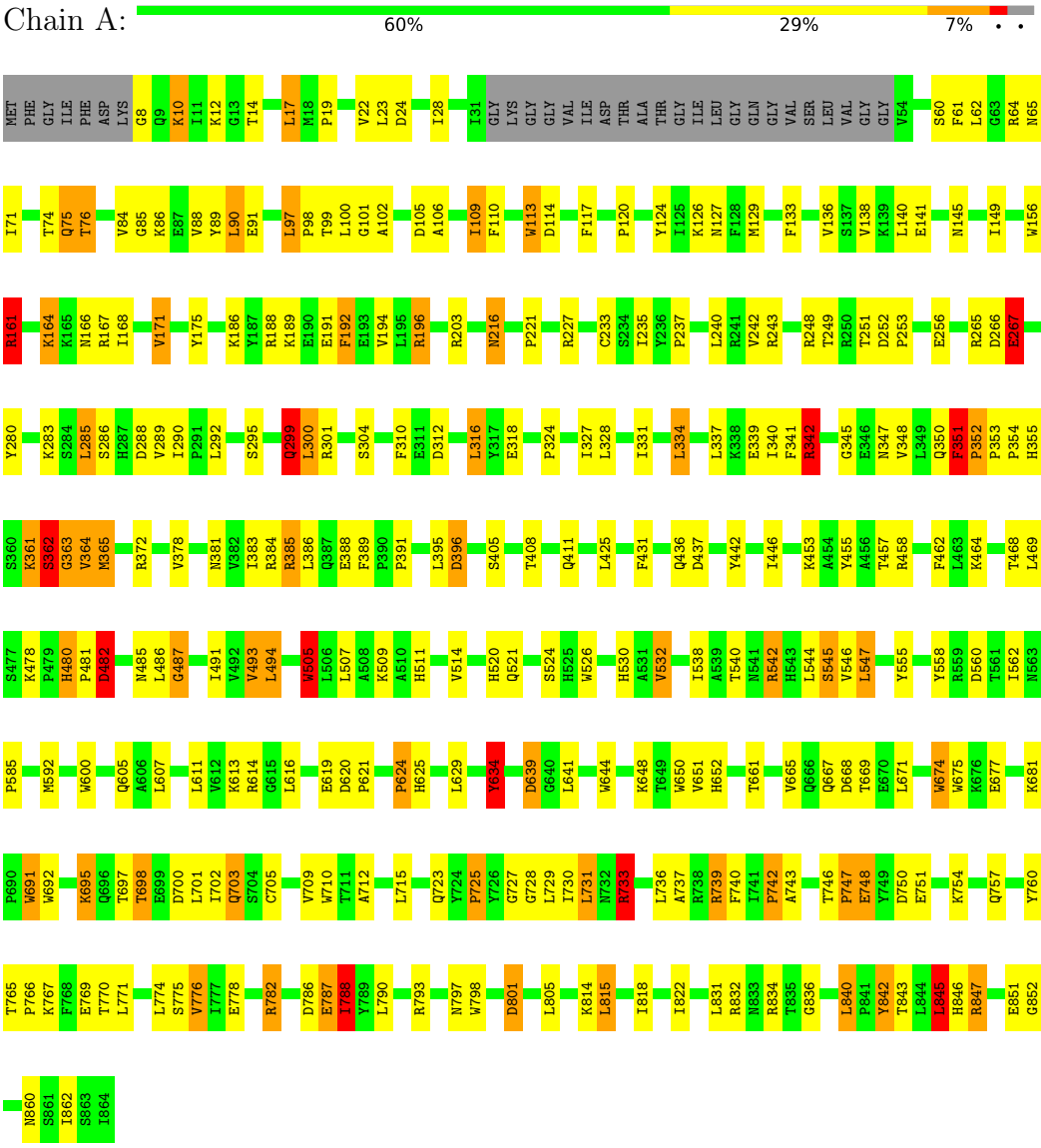
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

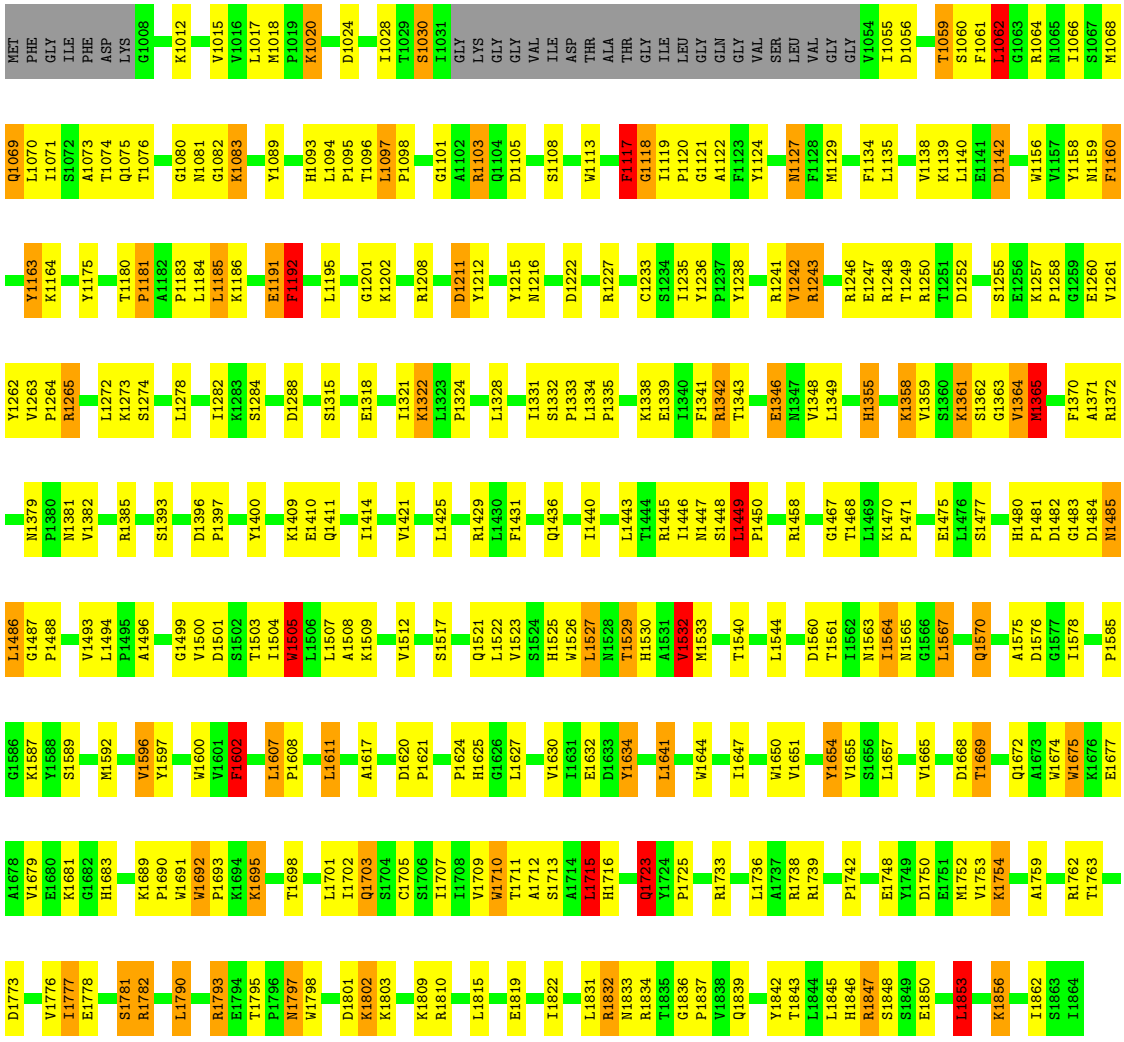
- Molecule 1: SEED LIPOXYGENASE

Chain A:



- Molecule 1: SEED LIPOXYGENASE

Chain B:


MET G1008 K1012 V1015 V1016 L1017 M1018 P1019 K1020 D1024 I1028 T1029 S1030 I1031 GLY LYS GLY GLY VAL ILE ASP THR ALA THR GLY ILE LEU GLY GLN GLY VAL SER LEU VAL GLY GLY V1054 I1055 D1056 T1059 S1060 F1061 L1062 G1063 R1064 N1065 I1066 S1067 M1068
Q1069 L1070 I1071 S1072 A1073 T1074 Q1075 T1076 G1080 N1081 G1082 K1083 Y1089 H1093 L1094 P1095 T1096 L1097 P1098 G1101 A1102 R1103 Q1104 D1105 S1108 W1113 F1117 G1118 I1119 P1120 G1121 A1122 F1123 Y1124 N1127 F1128 M1129 F1134 L1135 V1138 K1139 L1140 E1141 D1142 W1156 V1157 Y1158 N1159 F1160
Y1163 K1164 Y1175 T1180 P1181 A1182 P1183 L1184 L1185 K1186 E1191 F1192 L1195 G1201 K1202 R1208 D1211 Y1212 Y1215 N1216 D1222 R1227 C1233 S1234 I1235 Y1236 P1237 Y1238 R1241 V1242 R1243 R1246 E1247 R1248 T1249 R1250 T1251 D1252 S1255 E1256 K1257 P1258 G1259 E1260 V1261
Y1262 V1263 P1264 R1265 L1272 K1273 S1274 L1278 I1282 K1283 S1284 D1288 S1315 E1318 I1321 K1322 L1323 P1324 L1328 I1331 S1332 P1333 L1334 P1335 K1338 E1339 I1340 F1341 R1342 T1343 E1346 N1347 V1348 L1349 H1355 K1358 V1359 S1360 K1361 S1362 G1363 V1364 M1365 F1370 A1371 R1372
N1379 P1380 N1381 V1382 R1385 S1393 D1396 P1397 Y1400 K1409 E1410 Q1411 I1414 V1421 L1425 R1429 L1430 F1431 Q1436 I1440 L1443 T1444 R1445 I1446 N1447 S1448 L1449 P1450 R1458 G1467 T1468 L1469 K1470 P1471 E1475 L1476 S1477 H1480 P1481 D1482 G1483 D1484 N1485
L1486 G1487 P1488 V1493 L1494 P1495 A1496 G1499 V1500 D1501 S1502 T1503 I1504 W1505 L1506 L1507 A1508 K1509 V1512 S1517 Q1521 L1522 V1523 S1524 H1525 W1526 L1527 N1528 T1529 H1530 A1531 V1532 M1533 T1540 L1544 D1560 T1561 I1562 N1563 I1564 N1565 G1566 L1567 Q1570 A1575 D1576 G1577 I1578 P1585
G1586 K1587 Y1588 S1589 M1592 V1596 Y1597 W1600 V1601 F1602 L1607 P1608 L1611 A1617 D1620 P1621 P1624 H1625 G1626 L1627 V1630 I1631 E1632 D1633 Y1634 L1641 W1644 I1647 W1650 V1651 Y1654 V1655 S1656 L1657 V1665 D1668 T1669 Q1672 A1673 W1674 W1675 K1676 E1677
A1678 V1679 E1680 K1681 G1682 H1683 K1689 P1690 W1691 W1692 P1693 K1694 K1695 T1698 L1701 I1702 Q1703 S1704 C1705 S1706 I1707 I1708 V1709 W1710 T1711 A1712 S1713 A1714 L1715 H1716 Q1723 Y1724 P1725 R1733 L1736 A1737 R1738 R1739 P1742 E1748 Y1749 D1750 E1751 M1752 V1753 K1754 A1759 R1762 T1763
D1773 V1776 I1777 E1778 S1781 R1782 L1790 R1793 E1794 T1795 P1796 N1797 W1798 D1801 K1802 K1803 K1809 R1810 L1815 E1819 I1822 L1831 R1832 N1833 R1834 T1835 G1836 P1837 V1838 Q1839 Y1842 T1843 L1844 L1845 H1846 R1847 S1848 S1849 E1850 L1853 K1856 I1862 S1863 I1864

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.76Å 115.10Å 120.22Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.1 (50.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.84	3/6822 (0.0%)	1.66	136/9280 (1.5%)
1	B	0.83	1/6822 (0.0%)	1.58	92/9280 (1.0%)
All	All	0.84	4/13644 (0.0%)	1.62	228/18560 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	GLU	CB-CG	6.92	1.65	1.52
1	A	639	ASP	CA-CB	6.04	1.67	1.53
1	A	851	GLU	CG-CD	5.35	1.59	1.51
1	B	1798	TRP	CG-CD2	-5.23	1.34	1.43

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	362	SER	CA-C-N	-13.93	88.34	116.20
1	A	542	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	A	486	LEU	CA-C-N	-11.70	92.81	116.20
1	A	834	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	B	1793	ARG	NE-CZ-NH1	10.16	125.38	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PHE	Peptide
1	A	362	SER	Mainchain
1	A	480	HIS	Peptide
1	A	487	GLY	Peptide
1	A	97	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6649	0	6597	153	0
1	B	6649	0	6597	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	121	0	0	5	0
3	B	113	0	0	6	0
All	All	13534	0	13194	331	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 331 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HE	1:A:342:ARG:HA	1.31	0.94
1:A:847:ARG:NE	1:A:847:ARG:H	1.71	0.88
1:B:1020:LYS:H	1:B:1020:LYS:HD3	1.41	0.83
1:B:1371:ALA:HB2	1:B:1471:PRO:HD3	1.59	0.83
1:A:249:THR:HG22	1:A:252:ASP:H	1.43	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	831/864 (96%)	753 (91%)	58 (7%)	20 (2%)	6 6
1	B	831/864 (96%)	726 (87%)	77 (9%)	28 (3%)	3 3
All	All	1662/1728 (96%)	1479 (89%)	135 (8%)	48 (3%)	4 4

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	351	PHE
1	A	383	ILE
1	A	396	ASP
1	A	482	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	730/750 (97%)	643 (88%)	87 (12%)	5 6
1	B	730/750 (97%)	644 (88%)	86 (12%)	5 7
All	All	1460/1500 (97%)	1287 (88%)	173 (12%)	5 7

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1341	PHE

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Mol	Chain	Res	Type
1	B	1620	ASP
1	B	1364	VAL
1	B	1507	LEU
1	B	1703	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1485	ASN
1	B	1720	ASN
1	B	1528	ASN
1	B	1570	GLN
1	B	1797	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.